

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Database-restricted generation results for the NIST testing set in positive mode.

File Name: Supplementary Data 2

Description: Database-free generation results for the NIST testing set in positive mode.

File Name: Supplementary Data 3

Description: Metabolites annotation results across biological samples in positive mode.

File Name: Supplementary Data 4

Description: Database-restricted generation results for the NIST testing set in negative mode.

File Name: Supplementary Data 5

Description: Database-free generation results for the NIST testing set in negative mode.

File Name: Supplementary Data 6

Description: Metabolites annotation results across biological samples in negative mode.

File Name: Supplementary Data 7

Description: Compound information for the NIST testing set in positive mode.

File Name: Supplementary Data 8

Description: MS2 spectra across biological samples in positive mode.

File Name: Supplementary Data 9

Description: Compound information for the NIST testing set in negative mode.

File Name: Supplementary Data 10

Description: MS2 spectra across biological samples in negative mode.

File Name: Supplementary Data 11

Description: MS2 spectra in mouse liver dataset.

File Name: Supplementary Data 12

Description: Detailed compound information and annotation results of spike-in experiments.